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OPTIMAL DESIGNS FOR ESTIMATION OF THE TWO-PARAMETER LOGISTIC FU--ETC(U)

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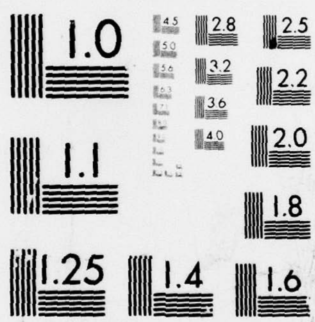

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OPTIMAL DESIGNS FOR ESTIMATION OF THE TWO-PARAMETER LOGISTIC FUNCTION

by

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I. INTRODUCTION

In this report optimal designs for weighted least squares and maximum likelihood estimation of the two-parameter logistic function are constructed[1]. First, some properties of the logistic function are discussed along with techniques for its estimation. Then, four criteria for optimality are defined and the corresponding optimal designs are constructed. Finally, some practical considerations in the implementation of these designs are mentioned.

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[1] A major portion of the research described in this report is based on the senior author's Masters paper [3] at the Pennsylvania State University. That paper, written under the direction of Dr. James L. Rosenberger of the Statistics Department, has been issued by that department as Technical Report No. 33 (August 1978).

II. THE LOGISTIC FUNCTION

The logistic function has the form

$$P = f(\underline{x}, \underline{\beta}) = [1 + \exp(-\underline{x}'\underline{\beta})]^{-1} \tag{1}$$

where $\underline{x} = (1, x_1, x_2, \ldots, x_k)'$ and $\underline{\beta} = (\beta_0, \beta_1, \beta_2, \ldots, \beta_k)'$. P takes on values in the interval (0, 1), $\underline{\beta}$ is the vector of parameters and $\underline{x}$ is the vector of independent (predictor) variables. The first element in $\underline{x}$, a "dummy variable", is included to provide for the estimation of an intercept.

This function is often used to describe the relationship between the vector $\underline{x}$ and the probability of a certain response, where the response is dichotomous. For example, the U.S. Navy's impact acceleration research program being conducted by the Naval Aerospace Medical Research Laboratory (NAMRL) Detachment is concerned with the relationships between various dynamic quantities (e.g., peak head linear acceleration and peak head angular acceleration) and the probability of injury. Here, $\underline{x}$ represents the values of the dynamic measurements and P is the corresponding probability of injury.

A. ESTIMATION OF THE LOGISTIC FUNCTION

Letting the n observations in an experiment be distinguished with the subscript i = 1, 2,...,n, the observed probability, denoted p_i, is given by

$$p_i = P_i + \varepsilon_i = f(\underline{x}_i, \underline{\beta}) + \varepsilon_i$$

where ε_i denotes the error term. Because of the binomial response (e.g., injury or noninjury) p_i is either 1 or 0. Therefore, ε_i is either $Q_i = 1 - P_i$ or $-P_i$ with corresponding probabilities P_i and Q_i respectively. From this it follows that

$$E(\varepsilon_i) = 0$$

$$\text{Var}\ (\varepsilon_i) = P_i Q_i$$

Since the error variances are not necessarily equal for different observations, it is appropriate to use weighted least squares to estimate $\underline{\beta}$.

It can be shown that the weighted least squares estimate of $\underline{\beta}$ is given by

$$\underline{b} = (\underline{X}'\underline{HX})^{-1}\ \underline{X}'\underline{Hy} \tag{2}$$

where $\underline{b}$ denotes the estimated parameter vector

$$\underline{b} = (\hat{\beta}_0, \hat{\beta}_1, \hat{\beta}_2, \ldots, \hat{\beta}_k)'; \tag{3}$$

$\underline{X}$ denotes the design matrix

$$\underline{X} = \begin{bmatrix} \underline{x}_1' \\ \underline{x}_2' \\ \cdot \\ \cdot \\ \cdot \\ \underline{x}_n' \end{bmatrix} ; \tag{4}$$

$\underline{H}$ denotes the diagonal weight matrix

$$\underline{H} = \begin{bmatrix} P_1Q_1 & & & & & \\ & P_2Q_2 & & & & \\ & & \cdot & & & \\ & & & \cdot & & \\ & & & & \cdot & \\ & & & & & P_nQ_n \end{bmatrix} ; \qquad (5)$$

and $\underline{y}$ denotes the vector of "working observations"

$$\underline{y} = (y_1, y_2, \ldots, y_n)' \qquad (6)$$

where $y_i = \frac{1}{P_iQ_i} [p_i - P_i + P_iQ_i \ln(P_i/Q_i)]$.

For a general discussion of weighted least squares, including a derivation of equation (2), see Draper and Smith [1]. Equation (2) is identical to that which would be obtained by maximum likelihood estimation. For a more complete mathematical development of the estimation process see Walker and Duncan [8] or Smith [7].[1]

Note that since $\underline{H}$ and $\underline{y}$ are functions of the probabilities $P_i = [1 + \exp(-\underline{x}'\underline{\beta})]^{-1}$, the estimate $\underline{b}$ in equation (2) must be obtained iteratively by using the values $\hat{P}_i = [1 + \exp(-\underline{x}'\underline{b})]^{-1}$ from the previous iteration. Because each observation (of injury or noninjury) corresponds

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[1] Equation (2) and definitions (3) through (6) are mathematically equivalent to the corresponding formulas given in the references [7, 8]. However, changes in notation were made so that formulas could be presented as they might be found in a standard textbook discussion of weighted least squares (such as Draper and Smith [1].)

to a value of $\hat{P}_i = p_i = 1$ or $\hat{P}_i = p_i = 0$, the actual observations cannot be used as initial estimates. This is not a major difficulty, and may be overcome by using initial estimates obtained by fitting a discriminant function. (See Jones [2].) An alternate recursive procedure (Walker and Duncan [8]) requires that initial estimates of the parameter vector and its covariance matrix be specified.

The asymptotic covariance matrix of $\underline{b}$ is

$$\mathrm{Var}(\underline{b}) = (\underline{X}'\underline{H}\underline{X})^{-1} . \tag{7}$$

In practical applications, the covariance matrix must be estimated by substituting

$$\hat{\underline{H}} = \begin{bmatrix} \hat{P}_1\hat{Q}_1 & & & \\ & \cdot & & \\ & & \cdot & \\ & & & \cdot \\ & & & & \hat{P}_n\hat{Q}_n \end{bmatrix}$$

for $\underline{H}$ into (7).

B. THE TWO-PARAMETER CASE

Since this report discusses optimal designs for the two-parameter case (k = 1), it will be convenient to introduce some additional notation and terminology for that special case. When k = 1, equation (1) is a sigmoid curve of the form

$$P = \{1 + \exp[-(\beta_0 + \beta_1 x)]\}^{-1} \tag{8}$$

and for $\beta_1 > 0$, P has asymptotic limits 0 and 1 as x approaches $-\infty$ and ∞ respectively. (See Figure 1.)

As an outgrowth of the early biological applications of the logistic function, x is often referred to as the "dose" and the level of x corresponding to a probability P of response is denoted LD_{100P}, where LD refers to "lethal dose." For example, a dose of amount LD_{75} would result in a response with probability .75. Designs for estimating the two-parameter logistic function are characterized in terms of LD levels at which observations are taken. For example, a typical design may allocate one quarter of the experimental units to LD_{10}, one half of the experimental units to LD_{50} and one quarter of the experimental units to LD_{90}.

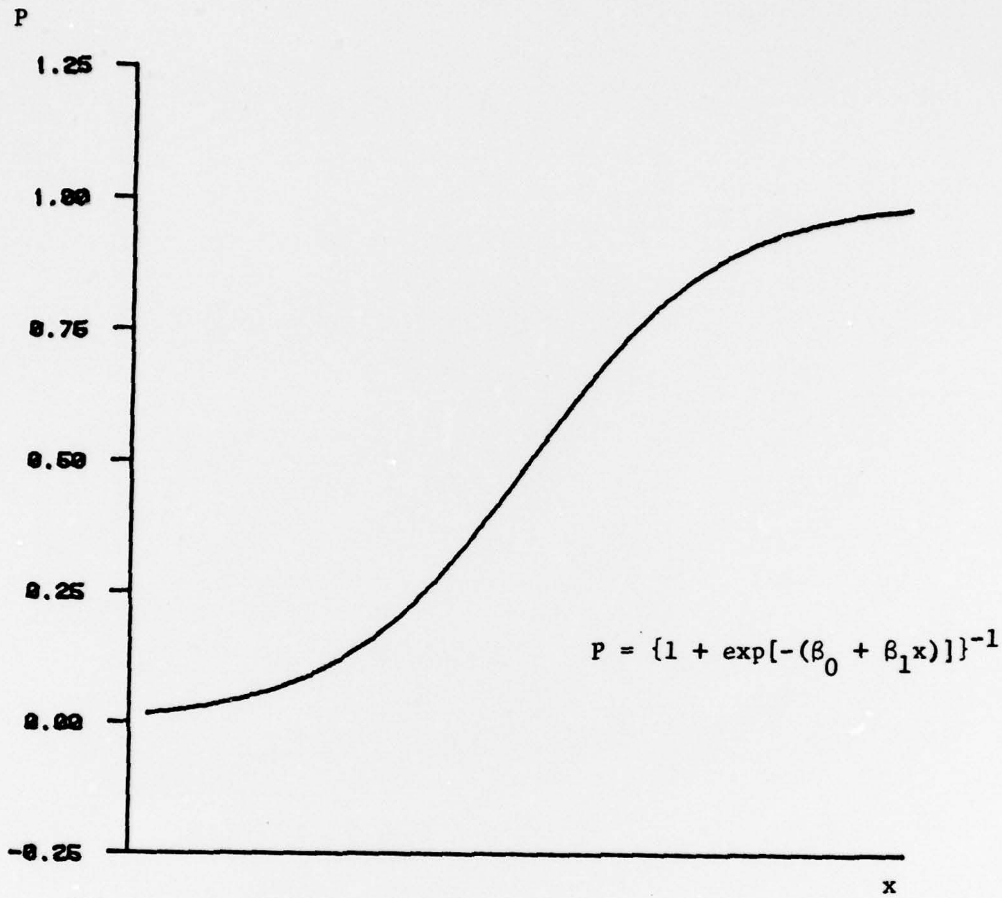

Figure 1: The two-parameter logistic function.

III. OPTIMAL DESIGNS

In general, an optimal design is one which "minimizes" the covariance matrix $(\underline{X}'\underline{HX})^{-1}$. The meaning of the word minimize, when applied to a matrix, is not obvious; a number of functionals of a covariance matrix have been proposed as criteria for minimization. For each criterion there is a corresponding optimal design. (See Kiefer [4].) These include:

1. D-optimality. Minimize by choice of design, the determinant of $(\underline{X}'\underline{HX})^{-1}$, denoted $|(\underline{X}'\underline{HX})^{-1}|$.

2. A-optimality. Minimize by choice of design, the trace of $(\underline{X}'\underline{HX})^{-1}$, denoted $\mathrm{tr}((\underline{X}'\underline{HX})^{-1})$.

3. E-optimality. Minimize, by choice of design, the maximum eigenvalue of $(\underline{X}'\underline{HX})^{-1}$.

4. G-optimality. Minimize, by choice of design, the maximum variance (over all dose levels x_0) of the predicted $\mathrm{var}(\hat{P}_0)$, where

$$\hat{P}_0 = \{1 + \exp[-(\hat{\beta}_0 + \hat{\beta}_1 x_0)]\}^{-1} .$$

These criteria are now examined more closely. Clearly, all of the information in an r x r covariance matrix needed by the D, A and E-optimality criteria is available in its eigenvalues, denoted $\lambda_1, \lambda_2, \ldots, \lambda_r$, since $|(\underline{X}'\underline{HX})^{-1}| = \prod_{i=1}^{r} \lambda_i$ and $\mathrm{tr}[(\underline{X}'\underline{HX})^{-1}] = \sum_{i=1}^{r} \lambda_i$. These three criteria can therefore be expressed (for the two-parameter case):

1. D-optimality. Minimize $(\lambda_1 \cdot \lambda_2)$.

2. A-optimality. Minimize $(\lambda_1 + \lambda_2)$.

3. E-optimality. Minimize max (λ_1, λ_2).

The determinant of $(\underline{X}'\underline{HX})^{-1}$, $|(\underline{X}'\underline{HX})^{-1}| = \lambda_1 \cdot \lambda_2$, is a general measure of the precision of the estimates $\hat{\beta}_0$ and $\hat{\beta}_1$. Note that $|(\underline{X}'\underline{HX})^{-1}| = \text{var}(\hat{\beta}_0)\text{var}(\hat{\beta}_1) - [(\text{cov}(\hat{\beta}_0, \hat{\beta}_1)]^2$. It will be shown that the D-optimal design is invariant to the choice of parameters or units of measurement of the dose.

The trace of $(\underline{X}'\underline{HX})^{-1}$, $\text{tr}[(\underline{X}'\underline{HX})^{-1}] = \lambda_1 + \lambda_2$, is not as general a measure of precision as $|(\underline{X}'\underline{HX})^{-1}|$, since the trace criterion ignores information about the covariance of $\hat{\beta}_0$ and $\hat{\beta}_1$. Note that $\text{tr}[(\underline{X}'\underline{HX})^{-1}] = \text{var}(\hat{\beta}_0) + \text{var}(\hat{\beta}_1)$. Furthermore, the A-optimal design is not invariant to the choice of parameters or units of measurement of the dose. The practical implications of this fact will be discussed in Section IV.

The maximum eigenvalue of $(\underline{X}'\underline{HX})^{-1}$, max (λ_1, λ_2), is the variance of that linear combination of $\hat{\beta}_0$ and $\hat{\beta}_1$ which is least precisely estimated by the design. Thus, E-optimality is a minimax criterion on the variance of all linear combinations of the estimated parameters. Since the set of eigenvalues gives all of the information contained in $(\underline{X}'\underline{HX})^{-1}$, some information is lost in ignoring the smaller eigenvalue. Like the A-optimal design, the E-optimal design is not invariant to the choice of parameters or units of measurement of the dose.

In considering the G-optimal design, it should be noted that the variance of a predicted value is a function not only of $(\underline{X}'\underline{HX})^{-1}$, but also of x_0, the dose at which the probability is being predicted. Furthermore,

the G-optimality criterion is a minimax criterion on the variance of a non-linear function of β_0 and β_1, namely the logistic function (8). Like the D-optimal design, the G-optimal design is invariant to the choice of parameters or units of measurement of the dose. It can be shown (Kiefer and Wolfowitz [5]) that the D-optimality and G-optimality criteria are equivalent for ordinary least squares estimation. (Recall that weighted least squares estimation is preferred for the logistic function.)

The four criteria discussed above are applicable regardless of the number of levels of x at which observations are taken. However, only two-point designs will be considered in this report for the following reasons. Sibson and Kenney [6] have shown that for ordinary least squares estimation, the D-optimal (and equivalently the G-optimal) designs for estimating r-order polynomial functions are (r + 1)-point designs. The logistic function (8) can be written as a first order polynomial as follows:

$$\ln[P/(1 - P)] = \beta_0 + \beta_1 x \ . \qquad (9)$$

The transformation by which the function (8) was linearized, $g(P) = \ln[P/(1 - P)]$, is often called the "logit" or "log odds ratio."

Although weighted least squares estimation is being used, it seems reasonable to believe that the optimal designs are two-point designs. Furthermore, since the logistic function is symmetric with respect to two rotations about $x = LD_{50}$ and $P = .50$ [that is, $f(LD_{100P}) = 1 - f(LD_{100(1-P)})$] only symmetric designs about LD_{50} with equal allocation to both design points will be considered.

Letting $Q' = 1 - P'$, the design points will be denoted $x_1 = LD_{100P'}$ and $x_2 = LD_{100Q'}$, where $P' > .50$. Thus, P' and Q' are the values of the

logistic function evaluated at design points x_1 and x_2 respectively. The sample size, denoted n, is assumed to be sufficiently large to use asymptotic theory.

Hence the symmetric two-point designs can be indexed simply by P'. If, for example, P' = .75, the design of the experiment would be to randomly allocate one half of the observations at $x_1 = LD_{75}$ and one half of the observations at $x_2 = LD_{25}$. (See Figure 2.)

Using the aforementioned notation and restrictions, $\underline{X}'\underline{HX}$ can be reduced to

$$\underline{X}'\underline{HX} = (n/2)P'Q'\begin{bmatrix} 2 & x_1 + x_2 \\ x_1 + x_2 & x_1^2 + x_2^2 \end{bmatrix} . \tag{10}$$

A. CONSTRUCTION OF D-OPTIMAL DESIGNS

The problem is to minimize $|(\underline{X}'\underline{HX})^{-1}|$ over choices of design. This is equivalent to maximizing $|\underline{X}'\underline{HX}|$, since for any nonsingular matrix A, $|A^{-1}| = 1/|A|$. Thus, the D-optimality criterion can be written $\max_{P'}|\underline{X}'\underline{HX}|$. Now from (10),

$$|\underline{X}'\underline{HX}| = [(n/2)P'Q'(x_1 - x_2)]^2. \tag{11}$$

But from (8) or (9),

$$x_1 = [\ln(P'/Q') - \beta_0]/\beta_1 \text{ and } x_2 = [\ln(Q'/P') - \beta_0]/\beta_1. \tag{12}$$

Substituting these equalities into (11),

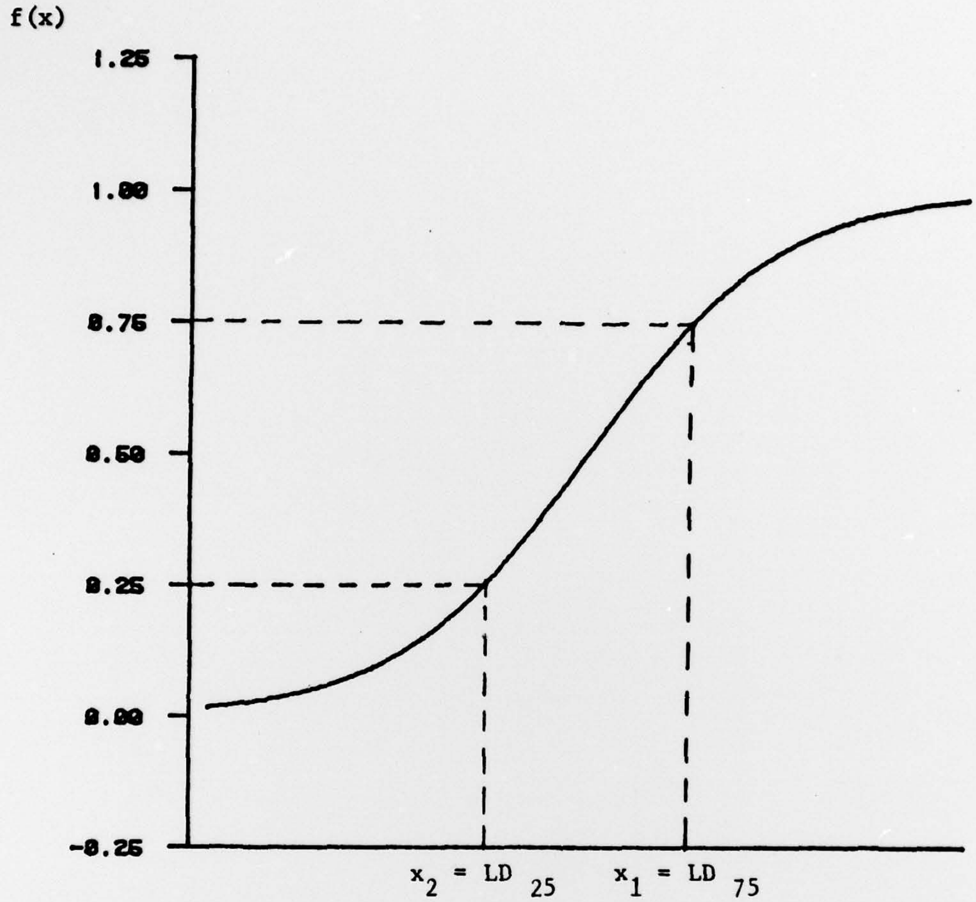

Figure 2: A symmetric two-point design with design points $x_1 = LD_{75}$ and $x_2 = LD_{25}$.

$$|\underline{X}'\underline{HX}| = [nP'Q'\ln(P'/Q')/\beta_1]^2. \tag{13}$$

So $\max_{P'}|\underline{X}'\underline{HX}| = \max_{P'}[nP'Q'\ln(P'/Q')/\beta_1]^2.$

To maximize, set the first partial derivative with respect to P' equal to zero. The solution to this can be numerically obtained as P' = .824, Q' = .176.

Thus, the two-point, symmetric about LD_{50}, D-optimal design is to allocate half of the experimental units to $LD_{82.4}$ and half of the experimental units to $LD_{17.6}$. Note that the optimal design is invariant to the choice of parameters, β_0 and β_1, or units of measurement of the dose, x.

B. CONSTRUCTION OF A-OPTIMAL DESIGNS

The trace criterion specifies that $tr[(\underline{X}'\underline{HX})^{-1}]$ be minimized over choices of design. From (10) and (12) it can be shown (see Kalish [3]) that

$$tr[(\underline{X}'\underline{HX})^{-1}] = 1/nP'Q' + (\beta_0^2 + \beta_1^2)/\{nPQ[\ln(P'/Q')]\}^2$$

To minimize, set the first partial derivative with respect to P' equal to zero. The solution is not invariant to the choice of β_0 and β_1. In fact, the A-optimal design depends on the sum of the squares of the parameters (i.e., on $\beta_0^2 + \beta_1^2$). A-optimal designs were constructed for several choices of parameters, using a computerized numerical search approach (see Kalish [3]). Figure 3 shows the relationship between the A-optimal design (indexed by P') and $\beta_0^2 + \beta_1^2$. Note that as $\beta_0^2 + \beta_1^2$ gets larger, the design points move outward from LD_{50}. In fact, their asymptotic limits (as $\beta_0^2 + \beta_1^2$ approaches ∞) are $LD_{91.7}$ and $LD_{08.3}$.

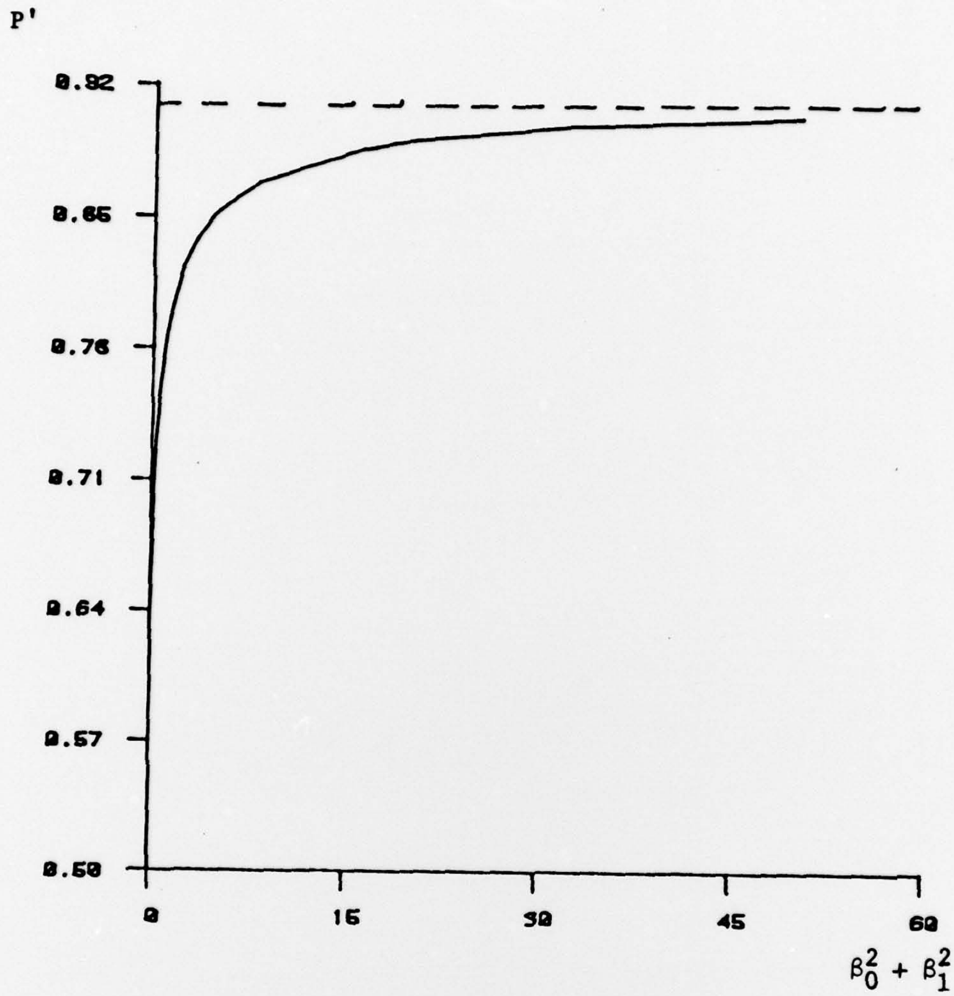

Figure 3: A-optimal designs (indexed by P') as a function of $\beta_0{}^2 + \beta_1{}^2$.

C. CONSTRUCTION OF E-OPTIMAL DESIGNS

For this criterion, the maximum eigenvalue of $(\underline{X}'\underline{HX})^{-1}$ is minimized over choices of design. Recall that the eigenvalues of a k x k matrix, $\underline{M}$, are the k roots of the equation $|\underline{M} - \lambda \underline{I}_k| = 0$, where $\underline{I}_k$ denotes the identity matrix of order k. It can be shown (see Kalish [3]) that the maximum eigenvalue is given by

$$\max(\lambda_1, \lambda_2) = \frac{\beta_0^2 + \beta_1^2 + (\ln(P'/Q'))^2 + \sqrt{[\beta_0^2 + \beta_1^2 + (\ln(P'/Q'))^2]^2 - [2\beta_1 \ln(P'/Q')]^2}}{2\,nP'Q'(\ln(P'/Q'))^2}.$$

The problem of minimizing this equation with respect to P' was approached analytically but the calculations became intractable. Thus, a computerized numerical search was used (see Kalish [3]). As with the A-optimal designs, the E-optimal design points move outward towards $LD_{91.7}$ and $LD_{08.3}$ as the parameters get larger. In this case, however, P' is not a monotone function of $\beta_0^2 + \beta_1^2$.

D. CONSTRUCTION OF G-OPTIMAL DESIGNS

Recall that G-optimality is a minimax criterion on the variance of the predicted values. As before, denote the probabilities corresponding to design points $x_1 = LD_{100P'}$ and $x_2 = LD_{100(1-P')}$ as P' and Q' respectively. Furthermore, refer to $\hat{P}_0$ as the predicted value corresponding to x_0. Using this notation, the G-optimality criterion can be expressed $\min_{P'} \max_{\hat{P}_0}[\mathrm{var}(\hat{P}_0)]$.

Note that $\mathrm{var}(\hat{P}_0)$ cannot be calculated directly since $\hat{P}_0$ is a nonlinear function of β_0 and β_1. However, using a Taylor series expansion, it can be shown that the asymptotic variance of $\hat{P}_0$ is

$$\mathrm{var}(\hat{P}_0) = \frac{(x_0 - x_1)^2 + (x_0 - x_2)^2}{(n/2)P'Q'(x_1 - x_2)^2} \, [e^{-L_0}/(1 + e^{-L_0})^2]^2,$$

where $L_0 = \ln[P_0/(1 - P_0)] = \beta_0 + \beta_1 x_0$. This can be further simplified to be written only in terms of n, P_0, P' (and $Q_0 = 1 - P_0$, $Q' = 1 - P'$) as

$$\mathrm{var}(\hat{P}_0) = \frac{[\ln(P_0Q'/Q_0P')]^2 + [\ln(P_0P'/Q_0Q')]^2}{(n/2)P'Q'[\ln(P^2/Q^2)]^2} \, [P_0Q_0]^2 .$$

The fact that $\mathrm{var}(\hat{P}_0)$ can be expressed as a function only of P_0 and the design (indexed by n and P) shows that the G-optimal design must be independent of the parameters β_0 and β_1. Thus, the G-optimality criterion is invariant to the choice of parameters or units of measurement of the dose.

An analytic approach to the minimax problem was attempted but again the calculations became intractable. Thus, a computerized numerical search was used (see Kalish [3]). It was found that the G-optimal design has design points at $x_1 = LD_{76.8}$ and $x_2 = LD_{23.2}$.

IV. PRACTICAL CONSIDERATIONS

The practical applications of the optimal designs discussed here require several considerations. One problem lies in the fact that the specification of an optimal design is done in terms of LD levels, yet in the design stage of an experiment, the LD levels are typically not known. Obviously, if a substantial amount of prior knowledge is available before experimentation, this can be used to give estimates of LD levels and of parameter values in order to approximate an optimal design.

If little or no prior information is available, a small pre-study experiment might be conducted wherein experimental units are allocated to some "reasonable" range of doses expected to cover the LD_{05} to LD_{95} levels. Data from the pre-study can then be used to estimate parameters and optimal design points. Of course, the pre-study data can later augment the primary experimental data to obtain final estimates.

Another practical problem to be resolved is which optimality criterion to use. It has already been mentioned that the D-optimal and G-optimal designs are invariant to choice of parameters, while the A-optimal and E-optimal designs are not. Since the values of a parameter are interpreted in the same units as x, any change in the scale of measurement of x would result in different A-optimal or E-optimal designs. For example, if velocity (x) were measured in meters per second, the A and E-optimal designs would differ from the A and E-optimal designs, respectively, if velocity were measured in centimeters per second.

Furthermore, it has been noted that the A and E-optimality criteria

do not use all of the information contained in $(\underline{X}'\underline{HX})^{-1}$. The trace criterion considers only the diagonal elements, $var(\hat{\beta}_0)$ and $var(\hat{\beta}_1)$, of the covariance matrix but not the off-diagonal elements, $cov(\hat{\beta}_0, \hat{\beta}_1)$. The maximum eigenvalue criterion utilizes the variance of only one of two orthogonal linear combinations of $\hat{\beta}_0$ and $\hat{\beta}_1$. For these reasons, the D-optimality and G-optimality criteria seem superior to the A-optimality and E-optimality criteria.

Assuming, then, that an experimenter has yet to choose between D and G-optimality, the following observation makes the decision seem less critical. Consider plots of these two criteria versus P'. Graphs of $|(\underline{X}'\underline{HX})^{-1}|$ versus P' and max $var(\hat{P}_0)$ versus P' are displayed in Figures 4 and 5. It can be seen that both curves are fairly flat for values of P' between .75 and .85. Due to the flatness of these curves in the region of the optimal designs (i.e., P' = .824 for D-optimality and P' = .768 for G-optimality), one can "miss" the optimal designs and still not sacrifice much efficiency in the estimation of the function. In fact, one can "almost" achieve optimality for both criteria simultaneously.

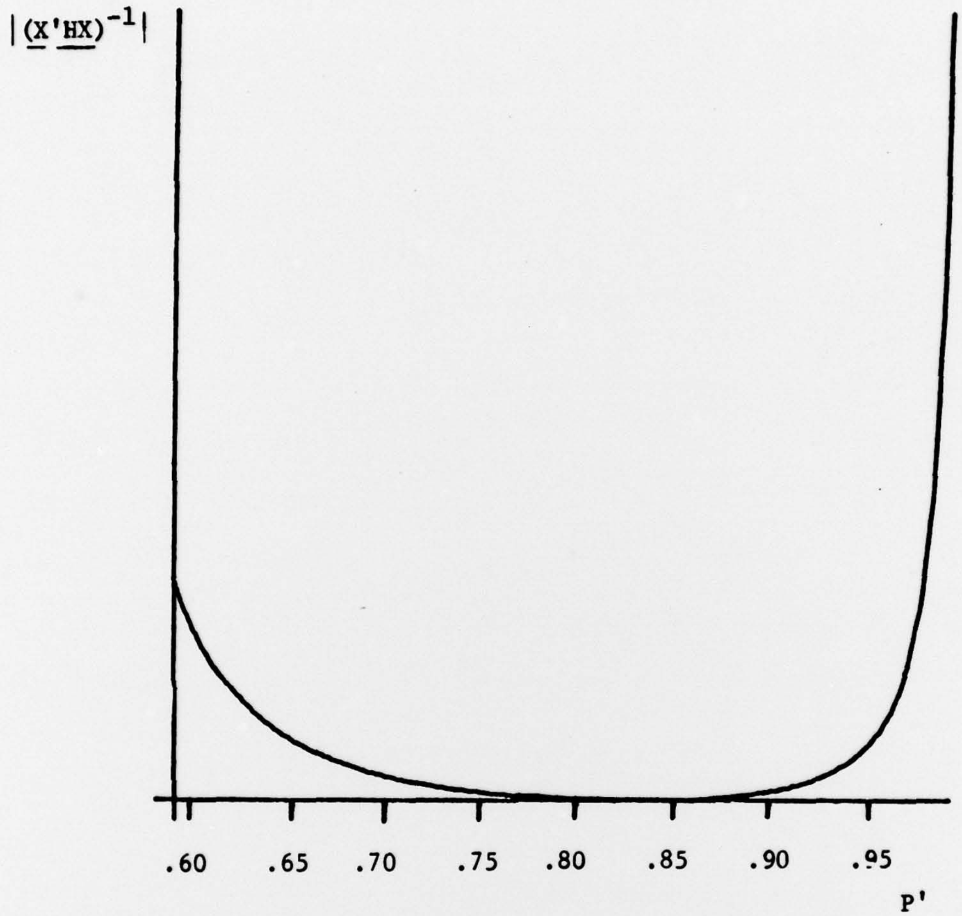

Figure 4: The D-optimality Criterion.

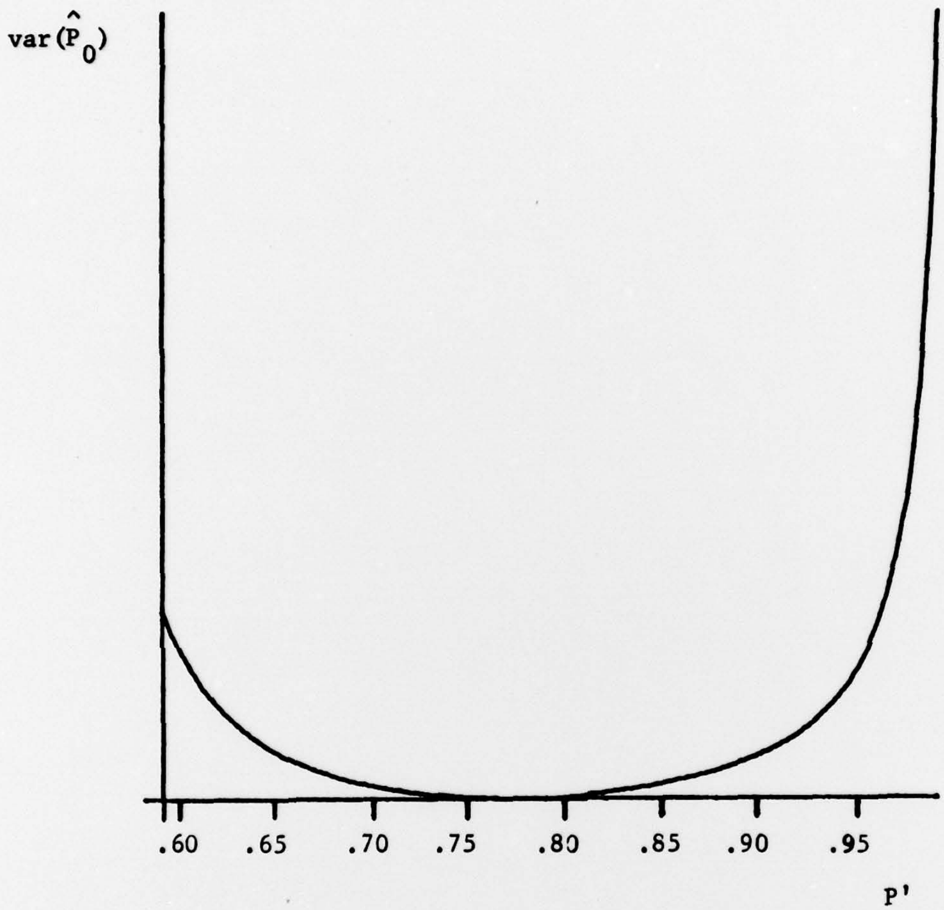

Figure 5: The G-optimality Criterion.

V. SUMMARY

In this report optimal designs were constructed for estimation of the two-parameter logistic function. In particular, four criteria for optimality were used: D, A, E and G-optimality. It was shown that the D and G-optimality criteria are invariant to changes in scale or units of measurement of the independent variable. In addition, the A and E-optimality criteria ignore some of the information available in the covariance matrix. For these reasons, the D and G-optimality criteria seem superior to the A and E-optimality criteria.

Since no criterion can be applied exactly in a real life setting, the problem of approximating an optimal design was briefly discussed. Two future technical reports will discuss an extension of this idea: that of augmenting an existing design one point at a time using an optimality criteria closely related to D-optimality.

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In this report, optimal designs for weighted least squares and maximum likelihood estimation of the two-parameter logistic function are constructed. In particular, four criteria for optimality are considered: D, A, E and G-optimality. The D and G-optimality criteria are found to be invariant to changes in scale while the A and E-optimality criteria are not. Practical problems which arise in the implementation of the optimal designs are discussed.

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